1-Methyl-6-(2-methylphenyl)-1,6-dihydro-3-pyridinecarbonitrile

27531-42-6 | DTXSID60299776

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 316 °C

Global applicability domain: Inside

Local applicability domain index: 3.94e-01

Confidence level: 5.34e-01

Nearest Neighbors from the Training Set

Image not found
Chlorothalonil
Measured: 350
Predicted: 319

Image not found
Acibenzolar-S-methyl
Measured: 267
Predicted: 295

Image not found
2-Methyl-5-nitro-1H-isoindole-1,3(2H)-dione
Measured: 361
Predicted: 323

Image not found
1-Phenylimidazole
Measured: 276
Predicted: 273

Image not found
1,5-Naphthalene diisocyanate
Measured: 330
Predicted: 319